

Pairing and the structure of the pf -shell $N \sim Z$ nuclei

Alfredo Poves[†] and Gabriel Martínez-Pinedo^{‡*}

[†]*Departamento de Física Teórica,*

Universidad Autónoma, Cantoblanco, 28049 Madrid, Spain

[‡] *W.K. Kellogg Radiation Laboratory, 106-38, California Institute of Technology
Pasadena, California 91125 USA*

(February 5, 2008)

The influence of the isoscalar and isovector $L = 0$ pairing components of the effective nucleon-nucleon interaction is evaluated for several isobaric chains, in the framework of full pf shell model calculations. We show that the combined effect of both isospin channels of the pairing force is responsible for the appearance of $T = 1$ ground states in $N = Z$ odd-odd nuclei. However, no evidence is found relating them to the Wigner energy. We study the dependence of their contributions to the total energy on the rotational frequency in the deformed nucleus ^{48}Cr . Both decrease with increasing angular momentum and go to zero at the band termination. Below the backbending their net effect is a reduction of the moment of inertia, more than half of which comes from the proton-neutron channel.

The study of the isovector pairing interaction among like particles is one of the classical themes of nuclear physics. Proton-neutron pairing, has been much less studied, in particular its isoscalar part. Early attempts to solve the isoscalar and isovector $L = 0$ pairing in one l shell can be found in ref. [1] and an extension to the two shells case in [2]. The experimental access to medium mass $N = Z$ nuclei, approaching the proton drip line has renewed the interest for the components of the nuclear interaction whose manifestations are enhanced close to $N = Z$. The proton-neutron part of the isovector pairing near $N = Z$ has been studied in term of algebraic model and compared with Shell Model Monte Carlo calculations in ref. [3].

In particular there are many discussions on the role of the isoscalar pairing interaction. Is it responsible for the Wigner energy? Should it give rise to a proton-neutron condensate? How will its manifestations evolve as the angular momentum increases?. Some of these issues have been examined in refs. [4,5]. The role of the isoscalar pairing channel in the processes mediated by the Gamow-Teller operator has been recently studied in ref. [6].

In this letter we take advantage of the availability of detailed microscopic descriptions of the nuclei in the middle of the pf -shell -that have already passed many experimental tests- to address some of these questions [7,8]. The existence of well deformed rotors in the $A = 50$ mass region makes it possible to explore the dependence of a given observable with the rotational frequency [9–12].

We shall study the isobaric chains $A = 46, 48$ and 50 , using the spherical shell model approach. The details of the shell model work have been explained in ref. [7]. We use the Lanczos shell model code ANTOINE (ref. [13]) and the effective interaction KB3. All the calculations presented are unrestricted in the pf -shell.

A key ingredient of our approach is the choice of the “physical” isoscalar and isovector pairing terms of the ef-

fective nuclear interaction. We follow here the work of Dufour and Zuker in ref [14], where they give a precise characterization of the multipole part of the nuclear interaction, showing in particular that the pairing term of any realistic G-matrix has only two contributions; the well known schematic isovector $L = 0, S = 0$ pairing and an isoscalar part which turns out to be again the schematic $L = 0, S = 1$ pairing. This eliminates many ambiguities associated to the choice of the isovector and isoscalar pairing interactions. We shall keep the notation in [14] and use P01 for the isovector and P10 for the isoscalar pairing. The explicit expressions for the two body matrix elements in LS and jj couplings are:

$$\begin{aligned} \langle l_A l_B LSJT | P01 | l_C l_D LSJT \rangle \\ = G \sqrt{(2l_A + 1)(2l_C + 1)} \delta_{AB} \delta_{CD} \delta_{L0} \delta_{S0} \delta_{J0} \delta_{T1}, \end{aligned} \quad (1a)$$

$$\begin{aligned} \langle l_A l_B LSJT | P10 | l_C l_D LSJT \rangle \\ = G \sqrt{(2l_A + 1)(2l_D + 1)} \delta_{AB} \delta_{CD} \delta_{L0} \delta_{S1} \delta_{J1} \delta_{T0}, \end{aligned} \quad (1b)$$

$$\begin{aligned} \langle j_a j_b JT | P01 | j_c j_d JT \rangle \\ = G \sqrt{(j_a + 1/2)(j_c + 1/2)} \delta_{ab} \delta_{cd} \delta_{J0} \delta_{T1}, \end{aligned} \quad (1c)$$

$$\begin{aligned} \langle j_a j_b JT | P10 | j_c j_d JT \rangle \\ = G \frac{2(-1)^{j_a - j_c}}{\sqrt{1 + \delta_{ab}} \sqrt{1 + \delta_{cd}}} \sqrt{(2j_a + 1)(2j_b + 1)(2j_c + 1)(2j_d + 1)} \\ \times \left\{ \begin{matrix} 1/2 & j_a & l_a \\ j_b & 1/2 & 1 \end{matrix} \right\} \left\{ \begin{matrix} 1/2 & j_c & l_c \\ j_d & 1/2 & 1 \end{matrix} \right\} \delta_{AB} \delta_{CD} \delta_{J1} \delta_{T0}, \end{aligned} \quad (1d)$$

where capital letters denote a l -orbit (quantum numbers nl) and lowercase letters denote a j -orbit (quantum numbers nj). The value for the pairing constant G is easily obtained from the numbers given in table I of the same reference. We use $G = -0.295$ for P01 and $G = -0.459$

for P10. It could be thinkable to do the same kind of analysis with a monopole free pairing interaction. We have verified that none of the conclusions of the paper would be modified if we did so. Thus, we decided to stick to the usual forms of pairing.

Once this definition of the pairing operators adopted, we focuss in the role they play in the behaviour of different nuclei and different physical quantities. For that we shall proceed in the most straightforward way; for each case we make first a reference calculation using the interaction KB3, then we subtract from KB3 the isovector or the isoscalar pairing hamiltonians and make the calculations with the new interactions KB3-P01 and KB3-P10. We obtain the effect of each pairing channel by direct comparison with the reference calculation. One could also estimate these effects in perturbation theory, in the cases studied here we have verified that the results are equivalent, however this may not be true in general.

Binding energies for an isobaric chain.

We begin with $A = 46$ in figure 1. We have plotted the contributions to the ground state binding energy (BE) from the isovector pairing (labeled P01) and from the isoscalar pairing (labeled P10). BE's are taken with the positive sign. The figure shows the strong odd-even staggering of the P01 points, mostly suppressed in the P10 case, as expected. The effect of P10, although important, is smaller than that of P01 and goes smoothly to zero as the number of valence protons goes to zero (notice that our description is fully simetric under the exchange of protons and neutrons). The only little surprise is that moving from $T = 1$ to $T = 0$, not only the contribution of P01 decreases, but also the contibution of P10, although to a lesser extent. This may explain why the ground state of ^{46}V has $T = 1$ instead of the expected $T = 0$. It goes like this; the monopole part of KB3 will put the centroid of the $T = 0$ states lower than the centroid of the $T = 1$ states by about 1.3 MeV; on the other hand, the total pairing contribution to $T = 1$ is larger by more than 1.5 MeV than the contribution to $T = 0$ (see figure 1), therefore it is finally the $T = 1$ state that becomes the ground state of the odd-odd $T_z = 0$ member of the multiplet. Notice that the inversion depends on the balance between the isovector monopole term and both pairings. As the isovector monopole has a smooth dependence with mass, while the isovector pairing depends linearly with the degeneracy of the orbit being filled, we expect the inversion to take place when high j orbits are dominant. When low j orbits are the relevant ones, the isoscalar pairing contribution to the $T = 0$ state can be enhanced due to the small spin-orbit splitting, what helps producing $T = 0$ ground states. This is borne out by the experiments; when the $1f_{7/2}$ orbit is being filled the $T = 1$ states are ground states, in ^{58}Cu the $2p_{3/2}$ orbit is dominant and restores a $T = 0$ ground state, in ^{62}Ga the influence of the $1f_{5/2}$ orbit shifts again to a

$T = 1$ ground state. From there on the $1g_{9/2}$ orbit starts to play an important role and $T = 1$ ground states occur in all cases. Actually the $T = 0$ - $T = 1$ splitting could give a hint on the ordering of the single particle orbits in places where no other information is available.

In figure 2 the same quantities are plotted for $A = 48$. The behaviour of the P10 contribution is very smooth and we do not find any breaking of slope at $T = 0$. The P01 points stagger as usual. In figure 3 we present $A = 50$. Now the part of the isobaric chain lying inside the pf -shell is longer and the trends seen in $A = 46$ better established. There is a slight increase of the P10 contribution from $T = 0$ to $T = 1$ followed by a smooth decrease, reaching zero at $T = 5$. As in $A = 46$ the reduction of both P10 and P01 contributions from $T = 1$ to $T = 0$ explains the occurrence of a $T = 1$ ground state in ^{50}Mn .

Wigner energy.

This name is given to the extra binding of the $T = 0$ member of an isobaric multiplet compared to what would be predicted by an $(N - Z)^2$ extrapolation from the other isobars. We can make an assesment of the role of the P01 and P10 terms proceeding as in the definition just given. In $A = 46$ we have too few nuclei in the valence space as to make the fit, therefore we only present results for the two other chains.

For $A = 48$,

$\epsilon_W = 2.82$	KB3
$\epsilon_W = 3.04$	KB3-P01
$\epsilon_W = 2.47$	KB3-P10

clearly the effect of both types of pairing on the Wigner energy is negligible.

For $A = 50$,

$\epsilon_W = 1.99$	KB3
$\epsilon_W = 2.60$	KB3-P01
$\epsilon_W = 2.12$	KB3-P10

the effect of the pairing terms is even less significant than in the $A = 48$ isobars. In conclusion, we find no link between the Wigner energy and the dominant pairing terms of the nuclear interaction. Furthermore, if we had made the fit with the more microscopic prescription $T(T + 1)$ the values of this "new" Wigner energy would have been much smaller (1.23 and 0.24 for $A = 48$ and $A = 50$) and the effect of the pairing terms negligible again. We therefore think that the Wigner energy cannot be explained as a pairing effect.

Pairing and angular momentum

The evolution of the pair content of a nucleus as the rotational frequency increases has been the subject of many

heated debates in the recent past. We have studied this evolution in several cases but we shall present only results for ^{48}Cr , which is the most representative example. In figure 4 we plot the contributions of the P10 and P01 pairing hamiltonians to the absolute energy of the yrast levels. Two regions show up, corresponding roughly to below/above the backbending. In the region of collective rotation the P01 contribution, that at $J = 0$ almost doubles the P10, decreases with J much more rapidly than the P10 one. At $J = 8$ both reach approximately the same value, and stay constant until they suddenly vanish at the aligned $J = 16$ state. In figure 5 we have translated the results of figure 4 to a backbending plot. The most visible effect of the pairing correlation is the well known reduction of the moment of inertia. The effect of the P01 channel is clearly dominant but the P10 contribution is far from being negligible and amounts to about one fourth of the P01. This suggests a plausible explanation to the discrepancies found in the comparison of the Cranked Hartree Fock Bogolyubov results using the Gogny force and the Shell Model (or the experimental ones) for the yrst band of ^{48}Cr [9]. Both approaches were shown to predict correctly the quadrupole properties, however the CHFB calculation gave a much larger moment of inertia. Actually it came out a factor three larger than the experiment, which is fully compatible with what we have seen to be the effect of taking out the proton neutron pairing ($T = 0$ and $T = 1$). Indeed, proton-neutron pairing is not properly taken into account in the standard HFB treatments. ^{50}Cr and ^{50}Mn behave in a qualitatively similar way. The only difference being the smaller role played by the P10 pairing in the moment of inertia of ^{50}Cr .

Pairing condensates?

There has been speculations recently on the possible existence of a new superfluid phase of nuclear matter made of a condensate of $L = 0$, $S = 1$ neutron proton pairs, that could be approachable in $N = Z$ nuclei. Once the meaning of “condensate” agreed, we can try to contribute to the debate.

Imagine that the $1f_{7/2}$ orbit were the valence space and P01 the effective interaction, in this case, the ground state of an even-even nucleus will be the seniority zero state that can be easily interpreted as a condensate of $L = 0$, $S = 0$, $T = 1$ pairs (with all the caveats, because only the valence particles are paired and the j 's of the orbits are not large enough compared with the number of active particles). Given that the $(1f_{7/2})^n$ configurations are the leading ones in the ground states of the nuclei we are interested in, it is in principle possible that the “P01 condensate”. i.e. the ground state of the $(1f_{7/2})^n$ isovector pairing problem, and the physical ground state could have a reasonable overlap. Furthermore, most of the properties of the $(1f_{7/2})^n$ pairing condensate persist if we solve the pairing problem in the full pf -shell with

the experimental single particle splitting.

On the contrary, if we solve the hamiltonian P10 in the $(1f_{7/2})^n$ configurations, we do not find any condensate. In order to obtain a condensate of $L = 0$, $S = 1$, $T = 0$ pairs, the valence space must include at least the $1f_{5/2}$ orbit degenerate with the $1f_{7/2}$, or, in general to be made of l -orbits, which is an extremely unphysical situation. Taking this argument to its limit one could say that the existence of a triplet pairing condensate is excluded by the spin orbit splitting of the nuclear mean field.

We have tried to make these statements quantitative computing the overlaps of the wave functions of the two condensates and the physical ground state in several pf -shell nuclei. Let's call $|\text{KB3}\rangle$ the physical ground state of a given nucleus obtained with the interaction KB3; $|\text{CP01}\rangle$ the isovector condensate obtained solving P01 in the pf shell with the experimental single particle splitting and $|\text{CP10}\rangle$ the isoscalar condensate obtained solving P10 in the pf shell without spin-orbit splitting, i.e. $l = 3$ and $l = 1$ separated by 2.0 MeV. The squared overlaps of these states with the physical ground state give the probabilities of finding the nuclei in the different condensed phases. The results are gathered in table I and the conclusions rather evident. The isovector $L = 0$ pairing condensate clearly dominates the structure of the Calcium isotopes we have selected. When two protons are added the overlaps get reduced and the interpretation in term of condensates is less justified. For the Chromiums no trace of a condensate is left. Notice that an overlap of 38% can be considered almost marginal. Actually, the overlap of the ^{48}Cr ground state, obtained using a pure $Q \cdot Q$ interaction and the isovector pairing condensate is already 25%. As anticipated the $L=0$ isoscalar pairing condensate does not show up, on the contrary it is almost exactly orthogonal to the physical ground states in most of the cases. As we said before, the existence of such a condensate would only be possible if in the valence space that accommodates the physics of the problem, the spin-orbit splittings were negligible.

Conclusions

We have explored the effect of the isovector and isoscalar $L = 0$ pairing interactions on several properties of pf -shell nuclei close to $N = Z$. We have found that the isoscalar pairing, whose contribution to the ground state binding energy of the nuclei studied may be very important, is not at the origin of the Wigner energy. Nor the isovector term. We argue that the occurrence of $T = 1$ ground states in odd-odd, $N = Z$ nuclei is due to the combined action of the two pairing channels that, when the dominant orbit has large l , can overcome the isovector monopole gap. We stress the need of a good treatment of the proton-neutron pairing in order to obtain the correct moment of inertia of $N = Z$ rotors. Finally we discard the presence of isoscalar pairing condensates everywhere in the region, as well as the existence of isovector pairing

condensates at $N = Z$.

ACKNOWLEDGMENTS

The authors thank P. Vogel, K. Langanke, S. Koonin, E. Caurier and A. Zuker for many interesting discussions. G.M. thanks the Spanish Ministerio de Educacion y Ciencia for a postdoctoral fellowship. This work has been partly supported by a grant of DGES (Spain) PB96-053.

-
- * Present address: Institute of Physics and Astronomy, University of Århus, DK-8000 Århus C, Denmark
- [1] J. A. Evans, G. G. Dussel, E. E. Maqueda and R. P. J. Perazzo, Nucl. Phys. **A367**, 77 (1981).
 - [2] G. G. Dussel, E. E. Maqueda, R. P. J. Perazzo and J. A. Evans, Nucl. Phys. **A460**, 164 (1986).
 - [3] J. Engel, K. Langanke and P. Vogel, Phys. Lett **B389**, 211 (1996).
 - [4] W. Satula, D. J. Dean, J. Gary, S. Mizutori and W. Nazarewicz, Phys. Lett. **B407**, 103 (1997).
 - [5] J. Terasaki, R. Wyss and P. H. Heenen, private communication.
 - [6] J. Engel, S. Pittel, M. Stoisov, P. Vogel and J. Dukelsky, Phys. Rev. **C 55**, 1781 (1997).
 - [7] E. Caurier, A. P. Zuker, A. Poves, and G. Martínez-Pinedo, Phys. Rev. C **50**, 225 (1994).
 - [8] G. Martínez-Pinedo, A. P. Zuker, A. Poves and E. Caurier, Phys. Rev. C. **55**, 187 (1997).
 - [9] E. Caurier, J. L. Egido, G. Martínez-Pinedo, A. Poves, J. Retamosa, L. M. Robledo and A. P. Zuker, Phys. Rev. Lett. **75**, 2466 (1995).
 - [10] G. Martínez-Pinedo, A. Poves, L. M. Robledo, E. Caurier, F. Nowacki, and A. P. Zuker, Phys. Rev. C **54**, R2150 (1996).
 - [11] S. Lenzi *et al.*, Z. Phys. **A354**, 117 (1996).
 - [12] S. Lenzi *et al* Phys. Rev. C **56**, 1313 (1997).
 - [13] E. Caurier, code ANTOINE, Strasbourg 1990.
 - [14] M. Dufour et A.P. Zuker, Phys. Rev. C **54**, 1641 (1996).

TABLE I. Overlaps between the physical ground state and the singlet and triplet pairing “condensates” in several nuclei.

nucleus	$ \langle \text{KB3} \text{CP01} \rangle ^2$	$ \langle \text{KB3} \text{CP10} \rangle ^2$	$ \langle \text{CP10} \text{CP01} \rangle ^2$
⁴⁴ Ca	97	-	-
⁴⁶ Ca	95	-	-
⁴⁴ Ti	63	16	1
⁴⁶ Ti	52	10	1
⁴⁸ Ti	59	1	0
⁴⁸ Cr	38	2	0
⁵⁰ Cr	42	1	0

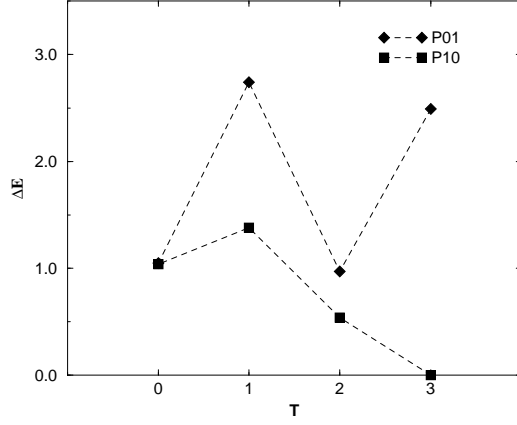


FIG. 1. Pairing contributions to the ground state energies of the $A=46$ isobaric multiplet (in MeV)

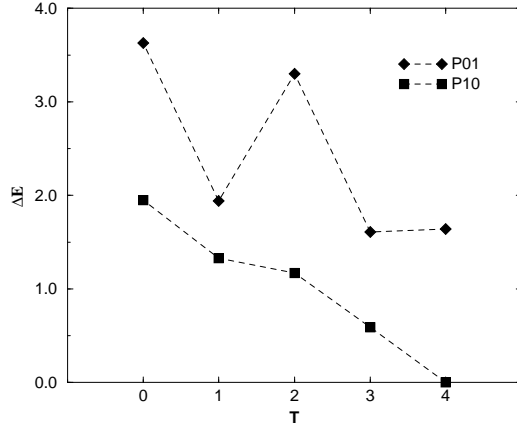


FIG. 2. Pairing contributions to the ground state energies of the $A=48$ isobaric multiplet (in MeV)

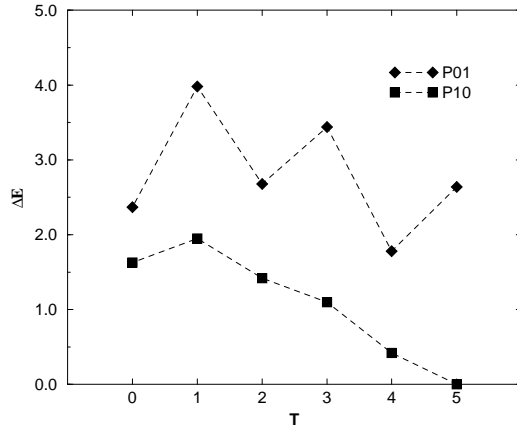


FIG. 3. Pairing contributions to the ground state energies of the $A=50$ isobaric multiplet (in MeV)

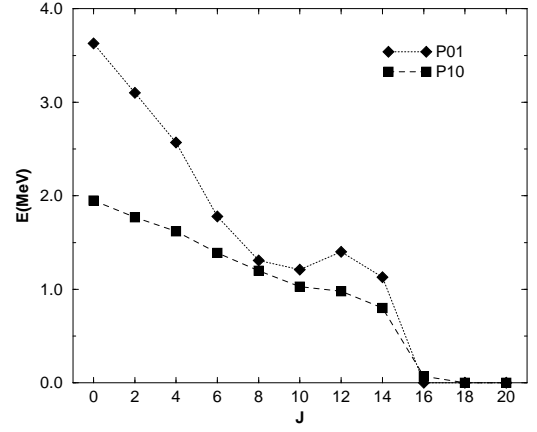


FIG. 4. Pairing contributions to the energies of the yrast states in ^{48}Cr .

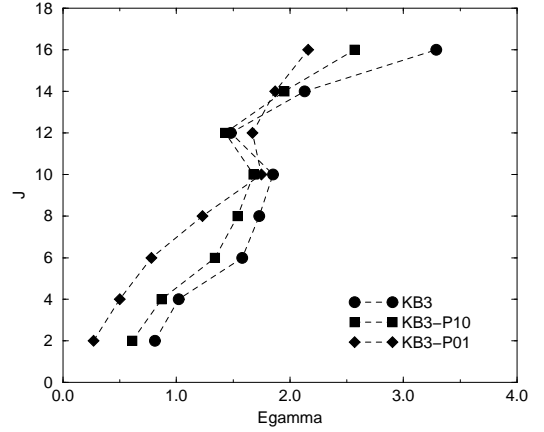


FIG. 5. Gamma ray energies along the yrast band of ^{48}Cr (in MeV); full interaction (KB3); without isoscalar pairing (KB3-P10); without isovector pairing (KB3-P01)